

SEQUENCE LISTING

<110> Xiaoling Xie

<120> CRYSTAL STRUCTURES OF JNK-INHIBITOR COMPLEXES AND
BINDING POCKETS THEREOF

<130> VPI/02-01

<140>

<141>

<150> 60/348,002

<151> 2002-01-11

<160> 7

<170> PatentIn Ver. 2.1

<210> 1

<211> 422

<212> PRT

<213> Homo sapiens

<400> 1

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Met Ser Leu His Phe Leu Tyr Tyr Cys Ser Glu Pro Thr Leu Asp Val
 1          5          10          15
Lys Ile Ala Phe Cys Gln Gly Phe Asp Lys Gln Val Asp Val Ser Tyr
          20          25          30
Ile Ala Lys His Tyr Asn Met Ser Lys Ser Lys Val Asp Asn Gln Phe
          35          40          45
Tyr Ser Val Glu Val Gly Asp Ser Thr Phe Thr Val Leu Lys Arg Tyr
          50          55          60
Gln Asn Leu Lys Pro Ile Gly Ser Gly Ala Gln Gly Ile Val Cys Ala
          65          70          75          80
Ala Tyr Asp Ala Val Leu Asp Arg Asn Val Ala Ile Lys Lys Leu Ser
          85          90          95
Arg Pro Phe Gln Asn Gln Thr His Ala Lys Arg Ala Tyr Arg Glu Leu
          100          105          110
Val Leu Met Lys Cys Val Asn His Lys Asn Ile Ile Ser Leu Leu Asn
          115          120          125
Val Phe Thr Pro Gln Lys Thr Leu Glu Glu Phe Gln Asp Val Tyr Leu
          130          135          140
Val Met Glu Leu Met Asp Ala Asn Leu Cys Gln Val Ile Gln Met Glu
          145          150          155          160
Leu Asp His Glu Arg Met Ser Tyr Leu Leu Tyr Gln Met Leu Cys Gly
          165          170          175
Ile Lys His Leu His Ser Ala Gly Ile Ile His Arg Asp Leu Lys Pro
          180          185          190
Ser Asn Ile Val Val Lys Ser Asp Cys Thr Leu Lys Ile Leu Asp Phe
          195          200          205

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Gly Leu Ala Arg Thr Ala Gly Thr Ser Phe Met Met Thr Pro Tyr Val
 210 215 220
 Val Thr Arg Tyr Tyr Arg Ala Pro Glu Val Ile Leu Gly Met Gly Tyr
 225 230 235 240
 Lys Glu Asn Val Asp Ile Trp Ser Val Gly Cys Ile Met Gly Glu Met
 245 250 255
 Val Arg His Lys Ile Leu Phe Pro Gly Arg Asp Tyr Ile Asp Gln Trp
 260 265 270
 Asn Lys Val Ile Glu Gln Leu Gly Thr Pro Cys Pro Glu Phe Met Lys
 275 280 285
 Lys Leu Gln Pro Thr Val Arg Asn Tyr Val Glu Asn Arg Pro Lys Tyr
 290 295 300
 Ala Gly Leu Thr Phe Pro Lys Leu Phe Pro Asp Ser Leu Phe Pro Ala
 305 310 315 320
 Asp Ser Glu His Asn Lys Leu Lys Ala Ser Gln Ala Arg Asp Leu Leu
 325 330 335
 Ser Lys Met Leu Val Ile Asp Pro Ala Lys Arg Ile Ser Val Asp Asp
 340 345 350
 Ala Leu Gln His Pro Tyr Ile Asn Val Trp Tyr Asp Pro Ala Glu Val
 355 360 365
 Glu Ala Pro Pro Pro Gln Ile Tyr Asp Lys Gln Leu Asp Glu Arg Glu
 370 375 380
 His Thr Ile Glu Glu Trp Lys Glu Leu Ile Tyr Lys Glu Val Met Asn
 385 390 395 400
 Ser Glu Glu Lys Thr Lys Asn Gly Val Val Lys Gly Gln Pro Ser Pro
 405 410 415
 Ser Ala Gln Val Gln Gln
 420

<210> 2
 <211> 340
 <212> PRT
 <213> Homo sapiens

<400> 2
 Phe Tyr Arg Gln Glu Leu Asn Lys Thr Ile Trp Glu Val Pro Glu Arg
 1 5 10 15
 Tyr Gln Asn Leu Ser Pro Val Gly Ser Gly Ala Tyr Gly Ser Val Cys
 20 25 30
 Ala Ala Phe Asp Thr Lys Thr Gly Leu Arg Val Ala Val Lys Lys Leu
 35 40 45
 Ser Arg Pro Phe Gln Ser Ile Ile His Ala Lys Arg Thr Tyr Arg Glu
 50 55 60
 Leu Arg Leu Leu Lys His Met Lys His Glu Asn Val Ile Gly Leu Leu
 65 70 75 80

Asp Val Phe Thr Pro Ala Arg Ser Leu Glu Glu Phe Asn Asp Val Tyr
 85 90 95
 Leu Val Thr His Leu Met Gly Ala Asp Leu Asn Asn Ile Val Lys Cys
 100 105 110
 Gln Lys Leu Thr Asp Asp His Val Gln Phe Leu Ile Tyr Gln Ile Leu
 115 120 125
 Arg Gly Leu Lys Tyr Ile His Ser Ala Asp Ile Ile His Arg Asp Leu
 130 135 140
 Lys Pro Ser Asn Leu Ala Val Asn Glu Asp Cys Glu Leu Lys Ile Leu
 145 150 155 160
 Asp Phe Gly Leu Ala Arg His Thr Asp Asp Glu Met Thr Gly Tyr Val
 165 170 175
 Ala Thr Arg Trp Tyr Arg Ala Pro Glu Ile Met Leu Asn Trp Met His
 180 185 190
 Tyr Asn Gln Thr Val Asp Ile Trp Ser Val Gly Cys Ile Met Ala Glu
 195 200 205
 Leu Leu Thr Gly Arg Thr Leu Phe Pro Gly Thr Asp His Ile Asp Gln
 210 215 220
 Leu Lys Leu Ile Leu Arg Leu Val Gly Thr Pro Gly Ala Glu Leu Leu
 225 230 235 240
 Lys Lys Ile Ser Ser Glu Ser Ala Arg Asn Tyr Ile Gln Ser Leu Thr
 245 250 255
 Gln Met Pro Lys Met Asn Phe Ala Asn Val Phe Ile Gly Ala Asn Pro
 260 265 270
 Leu Ala Val Asp Leu Leu Glu Lys Met Leu Val Leu Asp Ser Asp Lys
 275 280 285
 Arg Ile Thr Ala Ala Gln Ala Leu Ala His Ala Tyr Phe Ala Gln Tyr
 290 295 300
 His Asp Pro Asp Asp Glu Pro Val Ala Asp Pro Tyr Asp Gln Ser Phe
 305 310 315 320
 Glu Ser Arg Asp Leu Leu Ile Asp Glu Trp Lys Ser Leu Thr Tyr Asp
 325 330 335
 Glu Val Ile Ser
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<210> 3
 <211> 342
 <212> PRT
 <213> Homo sapiens

<400> 3
 Ala Gly Pro Glu Met Val Arg Gly Gln Val Phe Asp Val Gly Pro Arg
 1 5 10 15
 Tyr Thr Asn Leu Ser Tyr Ile Gly Glu Gly Ala Tyr Gly Met Val Cys
 20 25 30

Ser Ala Tyr Asp Asn Val Asn Lys Val Arg Val Ala Ile Lys Lys Ile
 35 40 45
 Ser Pro Phe Glu His Gln Thr Tyr Cys Gln Arg Thr Leu Arg Glu Ile
 50 55 60
 Lys Ile Leu Leu Arg Phe Arg His Glu Asn Ile Ile Gly Ile Asn Asp
 65 70 75 80
 Ile Ile Arg Ala Pro Thr Ile Glu Gln Met Lys Asp Val Tyr Ile Val
 85 90 95
 Gln Asp Leu Met Glu Thr Asp Leu Tyr Lys Leu Leu Lys Thr Gln His
 100 105 110
 Leu Ser Asn Asp His Ile Cys Tyr Phe Leu Tyr Gln Ile Leu Arg Gly
 115 120 125
 Leu Lys Tyr Ile His Ser Ala Asn Val Leu His Arg Asp Leu Lys Pro
 130 135 140
 Ser Asn Leu Leu Leu Asn Thr Thr Cys Asp Leu Lys Ile Cys Asp Phe
 145 150 155 160
 Gly Leu Ala Arg Val Ala Asp Pro Asp His Asp His Thr Gly Phe Leu
 165 170 175
 Thr Glu Tyr Val Ala Thr Arg Trp Tyr Arg Ala Pro Glu Ile Met Leu
 180 185 190
 Asn Ser Lys Gly Tyr Thr Lys Ser Ile Asp Ile Trp Ser Val Gly Cys
 195 200 205
 Ile Leu Ala Glu Met Leu Ser Asn Arg Pro Ile Phe Pro Gly Lys His
 210 215 220
 Tyr Leu Asp Gln Leu Lys His Ile Leu Gly Ile Leu Gly Ser Pro Ser
 225 230 235 240
 Gln Glu Asp Leu Asn Cys Ile Ile Asn Leu Lys Ala Arg Asn Tyr Leu
 245 250 255
 Leu Ser Leu Pro His Lys Asn Lys Val Pro Trp Asn Arg Leu Phe Pro
 260 265 270
 Asn Ala Asp Ser Lys Ala Leu Asp Leu Leu Asp Lys Met Leu Thr Phe
 275 280 285
 Asn Pro His Lys Arg Ile Glu Val Glu Gln Ala Leu Ala His Pro Tyr
 290 295 300
 Leu Glu Gln Tyr Tyr Asp Pro Ser Asp Glu Pro Ile Ala Glu Ala Pro
 305 310 315 320
 Phe Lys Phe Asp Met Glu Leu Asp Asp Leu Pro Lys Glu Lys Leu Lys
 325 330 335
 Glu Leu Ile Phe Glu Glu
 340

<210> 4
 <211> 256
 <212> PRT

<213> Mus musculus

<400> 4

Asp Gln Phe Asp Arg Ile Lys Thr Leu Gly Thr Gly Ser Phe Gly Arg
1 5 10 15
Val Met Leu Val Lys His Lys Glu Ser Gly Asn His Tyr Ala Met Lys
20 25 30
Ile Leu Asp Lys Gln Lys Val Val Lys Leu Lys Gln Ile Glu His Thr
35 40 45
Leu Asn Glu Lys Arg Ile Leu Gln Ala Val Asn Phe Pro Phe Leu Val
50 55 60
Lys Leu Glu Phe Ser Phe Lys Asp Asn Ser Asn Leu Tyr Met Val Met
65 70 75 80
Glu Tyr Val Ala Gly Gly Glu Met Phe Ser His Leu Arg Arg Ile Gly
85 90 95
Arg Phe Ser Glu Pro His Ala Arg Phe Tyr Ala Ala Gln Ile Val Leu
100 105 110
Thr Phe Glu Tyr Leu His Ser Leu Asp Leu Ile Tyr Arg Asp Leu Lys
115 120 125
Pro Glu Asn Leu Leu Ile Asp Gln Gln Gly Tyr Ile Gln Val Thr Asp
130 135 140
Phe Gly Phe Ala Lys Arg Val Lys Gly Arg Thr Trp Thr Leu Cys Gly
145 150 155 160
Thr Pro Glu Tyr Leu Ala Pro Glu Ile Ile Leu Ser Lys Gly Tyr Asn
165 170 175
Lys Ala Val Asp Trp Trp Ala Leu Gly Val Leu Ile Tyr Glu Met Ala
180 185 190
Ala Gly Tyr Pro Pro Phe Phe Ala Asp Gln Pro Ile Gln Ile Tyr Glu
195 200 205
Lys Ile Val Ser Gly Lys Val Arg Phe Pro Ser His Phe Ser Ser Asp
210 215 220
Leu Lys Asp Leu Leu Arg Asn Leu Leu Gln Val Asp Leu Thr Lys Arg
225 230 235 240
Phe Gly Asn Leu Lys Asp Gly Val Asn Asp Ile Lys Asn His Lys Trp
245 250 255

<210> 5

<211> 39

<212> DNA

<213> Artificial Sequence

<220>

<223> Description of Artificial Sequence: Primer

<400> 5

gctctagagc tccatgggca gcaaaagcaa agttgacaa

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<210> 6
<211> 37
<212> DNA
<213> Artificial Sequence

<220>
<223> Description of Artificial Sequence: Primer

<400> 6
tagcggatcc tcattctgaa ttcattactt ccttgta 37

<210> 7
<211> 21
<212> PRT
<213> Homo sapiens

<400> 7
Lys Arg Glu Leu Val Glu Pro Leu Thr Pro Ser Gly Glu Ala Pro Asn
1 5 10 15
Gln Ala Leu Leu Arg
20